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Diffusion for Weakly Coupled Quantum Oscillators

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Abstract. We construct a simple model which exhibits some of the properties discussed by van Hove in his study of the Pauli master equation. The model consists of an infinite chain of quantum oscillators which are coupled so that the interaction Hamiltonian is quadratic. We suppose the chain is in equilibrium at an inverse temperature β and study the return to equilibrium when a chosen oscillator is given an arbitrary perturbation. We show that in the limit as the interaction becomes weaker and of longer range, the evolution of the chosen oscillator becomes a diffusion equation. Moreover we give an explicit example where the evolution of the chosen oscillator has the Markov property and where the Pauli master equation is exactly satisfied.

§ 1. Introduction

We consider a linear chain of quantised harmonic oscillators interacting by a quadratic Hamiltonian in very much the same spirit as Ford, Kac and Mazur [1]. However, instead of taking a finite number $(2N+1)$ of oscillators and going to the limit $N\to\infty$, we take an infinite number of oscillators from the beginning, with an interaction which has a cut-off depending on a parameter $\lambda>0$, and go to the limit as $\lambda\to 0$.

We let the Hamiltonian of the system be

$$H_\lambda = H_0 + H_{I,\lambda} \tag{1.1}$$

where

$$H_0 = \tfrac{1}{2}\sum_{n=-\infty}^{\infty} :p_n^2+\omega^2 q_n^2: \tag{1.2}$$

and

$$H_{I,\lambda} = \sum_{m,n} :\alpha_{m-n}^{(\lambda)} q_m q_n: \tag{1.3}$$

For the time being we suppose only that $a_m^{(\lambda)}$ are real coefficients satisfying

$$\sum_{m=-\infty}^{\infty} |a_m^{(\lambda)}| < \infty \tag{1.4}$$

for all $\lambda>0$. The operators p_m and q_n are supposed to satisfy the commutation relations

$$[q_m, p_n] = i\delta_{mn}; \qquad [q_m, q_n] = [p_m, p_n] = 0\,. \tag{1.5}$$

We let

$$q_m = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{im\theta} \phi_0(\theta)\, d\theta; \qquad p_n = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{in\theta} \pi_0(\theta)\, d\theta \tag{1.6}$$

so that

$$H_0 = \tfrac{1}{2} \int_{-\pi}^{\pi} :\pi_0(\theta)^2 + \omega^2 \phi_0(\theta)^2 : d\theta \tag{1.7}$$

and

$$H_{I,\lambda} = \int_{-\pi}^{\pi} :B_\lambda(\theta)\, \phi_0(\theta)^2 : d\theta \tag{1.8}$$

where

$$B_\lambda(\theta) = \sum_{m=-\infty}^{\infty} a_m^{(\lambda)} e^{im\theta} \tag{1.9}$$

is a real, continuous, periodic function on $[-\pi, \pi]$.

We now suppose that

$$|B_\lambda(\theta)| \leqq \frac{c}{2} \tag{1.10}$$

for some constant $c < \omega^2$ which is independent of λ and θ and define

$$C_\lambda(\theta) = \{\omega^2 + 2 B_\lambda(\theta)\}^{\frac{1}{2}}. \tag{1.11}$$

For the present we drop the parameter λ for notational simplicity, and start making the above remarks more precise.

We take as a test function space M the real Hilbert space of all square integrable functions f on $[-\pi, \pi]$ such that $f(-\theta) = \overline{f(\theta)}$ almost everywhere. For any real index α we define the bounded self-adjoint operator $C^\alpha : M \to M$ by

$$(C^\alpha f)(\theta) = \{C(\theta)\}^\alpha f(\theta). \tag{1.12}$$

For any $f, g \in M$ we let $a^*(f)$ and $a(g)$ be the smeared creation and annihilation operators realised on Fock space, so that

$$[a(f), a^*(g)] = \langle f, g \rangle 1; \qquad [a(f), a(g)] = [a^*(f), a^*(g)] = 0. \tag{1.13}$$

We define the smeared fields at time zero by

$$\phi_0(f) = \frac{1}{\sqrt{2}} \{a^*(C^{-\frac{1}{2}} f) + a(C^{-\frac{1}{2}} f)\}, \tag{1.14}$$

$$\pi_0(g) = \frac{i}{\sqrt{2}} \{a^*(C^{\frac{1}{2}} g) - a(C^{\frac{1}{2}} g)\} \tag{1.15}$$

and note that the Hamiltonian H is given by

$$H = \int_{-\pi}^{\pi} C(\theta)\, a^*(\theta)\, a(\theta)\, d\theta \tag{1.16}$$

which it is not difficult to give a precise meaning as a self-adjoint operator on Fock space. As in [1] we then find that the time t fields are given by

$$\phi_t(f)=e^{iHt}\,\phi_0(f)\,e^{-iHt}=\phi_0\{\cos(Ct)\,f\}+\pi_0\{C^{-1}\sin(Ct)\,f\}\,, \tag{1.17}$$

$$\pi_t(g)=e^{iHt}\,\pi_0(g)\,e^{-iHt}=-\pi_0\{C\sin(Ct)\,g\}+\phi_0\{\cos(Ct)\,g\}\,. \tag{1.18}$$

The fields are easy to define as self-adjoint operators and we write

$$U(f,g)=\exp[i\phi_0(f)+i\pi_0(g)] \tag{1.19}$$

so that these unitary operators satisfy a form of the Weyl commutation relations.

We should now like to define the equilibrium state at the inverse temperature β as $\varrho=ke^{-\beta H}$ but this is not possible in the Fock representation because H has continuous spectrum. We overcome this difficulty by making use of expectation functions for the canonical commutation relations as in the paper of Araki and Woods [2]. They show that if $E_\beta : M\times M\to\mathbb{C}$ is defined by

$$E_\beta(f,g)=\exp\left[-\frac{1}{4}\left\langle C^{-1}\coth\left(\frac{\beta C}{2}\right)f,f\right\rangle-\frac{1}{4}\left\langle C\coth\left(\frac{\beta C}{2}\right)g,g\right\rangle\right]$$

then there is a representation of the canonical commutation relations over M with cyclic vector Ω_β such that

$$E_\beta(f,g)=\langle U(f,g)\,\Omega_\beta,\Omega_\beta\rangle\,. \tag{1.20}$$

We take this as the expectation function defining the equilibrium state at the inverse temperature β, noting that it satisfies the K.M.S. condition with respect to the time evolution [3]. In particular at zero temperature

$$E_\infty(f,g)=\exp[-\tfrac{1}{4}\|C^{-\frac{1}{2}}f\|^2-\tfrac{1}{4}\|C^{\frac{1}{2}}g\|^2] \tag{1.21}$$

and the representation may be realised on Fock space.

§ 2. Evolution of a Finite Subsystem

We study the evolution of the finite subsystem consisting of the oscillators indexed by $N(1),\ldots,N(n)$. To do this we let $e_r\in M$ be defined by

$$e_r(\theta)=\frac{1}{\sqrt{2\pi}}\,e^{iN(r)\theta} \tag{2.1}$$

and let L be the n-dimensional subspace of M generated by $e_1,\ldots,e_n$. The projection P of M onto L is given by

$$Pf=\sum_{r=1}^{n}\langle f,e_r\rangle\,e_r\,. \tag{2.2}$$

We suppose that just before time $t=0$ this finite subsystem has been given an arbitrary perturbation, and study its return to the equilibrium state. This is done most conveniently in the Heisenberg representation. We describe the evolution of the Weyl operators for all non-negative times t by the equation

$$\alpha_t\{U(x,y)\} = M\{e^{iHt}\, U(x,y)\, e^{-iHt}\} \tag{2.3}$$

where $x, y \in L$ and M denotes the operation of taking the expectation, with respect to the thermal equilibrium state, of all expressions involving the field operators for the oscillators other than those indexed by $N(1), \ldots, N(n)$. (The operation M will be described with more precision in Section 4, but its application in this context causes no difficulties.)

The following lemma makes hardly any use of the properties of our particular model and can be studied in a much more general context. This has been done, from a rather different point of view, by Lewis and Thomas [4, 5].

Lemma 2.1.
$$\alpha_t\{U(x,y)\} = U(x_t, y_t)\exp\left[-\tfrac{1}{4}r_t\right] \tag{2.4}$$

for all $x, y \in L$, where

$$x_t = P\cos(Ct)\,x - PC\sin(Ct)\,y\,, \tag{2.5}$$

$$y_t = PC^{-1}\sin(Ct)\,x + P\cos(Ct)\,y\,, \tag{2.6}$$

$$r_t = \left\langle C^{-1}\coth\left(\frac{\beta C}{2}\right)\xi_t, \xi_t\right\rangle + \left\langle C\coth\left(\frac{\beta C}{2}\right)\eta_t, \eta_t\right\rangle, \tag{2.7}$$

$$\xi_t = \cos(Ct)\,x - C\sin(Ct)\,y - x_t\,, \tag{2.8}$$

$$\eta_t = C^{-1}\sin(Ct)\,x + \cos(Ct)\,y - y_t\,. \tag{2.9}$$

Proof. We first note that $P\xi_t = P\eta_t = 0$ so that ξ_t and η_t do not depend on the states of the oscillators indexed by $N(1), \ldots, N(n)$. Simple calculations show that

$$e^{iHt}\{\phi_0(x)+\pi_0(y)\}\,e^{-iHt} = \phi_0(x_t)+\pi_0(y_t)+\phi_0(\xi_t)+\pi_0(\eta_t)$$

so

$$e^{iHt}\,U(x,y)\,e^{-iHt} = U(x_t, y_t)\cdot U(\xi_t, \eta_t)\,. \tag{2.10}$$

Our prescription for the operation M now yields

$$\alpha_t\{U(x,y)\} = U(x_t, y_t)\,E_\beta(\xi_t, \eta_t) \tag{2.11}$$

which is the expression given by the lemma.

We now return to the consideration of how the interaction depends on the parameter λ. Our first assumption, that the interaction becomes weaker as $\lambda \to 0$, is formulated precisely in the following lemma.

Lemma 2.2. *Suppose* $\lim_{\lambda\to 0} B_\lambda(\theta)=0$ *for almost every* $\theta\in[\pi\pi]$. *Then for all* $t>0$ *and all* $x, y\in L$

$$\lim_{\lambda\to 0}\alpha_{\lambda,t}\{U(x,y)\}=e^{iH_0t}\,U(x,y)\,t^{-iH_0t} \tag{2.12}$$

the limit being taken in the strong operator topology.

Proof. By our assumptions leading up to the definition of $C_\lambda(\theta)$ in Eq. (1.11) we see that $C_\lambda(\theta)$ is uniformly bounded, uniformly bounded away from zero and converges almost everywhere to ω. Repeated use of the Lebesgue dominated convergence theorem now leads to

$$x'_t\equiv\lim_{\lambda\to 0}x_{\lambda,t}=x\cos\omega t-y\omega\sin\omega t\,, \tag{2.13}$$

$$y'_t\equiv\lim_{\lambda\to 0}y_{\lambda,t}=x\omega^{-1}\sin\omega t+y\cos\omega t \tag{2.14}$$

and

$$\lim r_{\lambda,t}=0 \tag{2.15}$$

so that

$$\begin{aligned}\lim_{\lambda\to 0}\alpha_{\lambda,t}\{U(x,y)\}&=U(x'_t,y'_t)\\&=e^{iH_0t}\,U(x,y)\,e^{-iH_0t}\,.\end{aligned}$$

For computational convenience we transform the above equations to complex form. We define

$$z=\omega^{-\frac{1}{2}}x+i\omega^{\frac{1}{2}}y \tag{2.16}$$

so that

$$z'_t=e^{i\omega t}z\,. \tag{2.17}$$

The lemma suggests that as the interaction becomes weaker its effect on the evolution of the system becomes negligible. However, this need not be true. What can happen is that as $\lambda\to 0$ the rate of the interaction becomes slower, but if one waits long enough the cumulative effect need not be negligible. Mathematically the reason the above lemma is not conclusive is that the convergence is not uniform with respect to time.

In order to investigate this further, we introduce a new time parameter τ and suppose t is a function of τ and λ, namely

$$t=\lambda^{-2}\tau\,. \tag{2.18}$$

Compare van Hove's change of time scale [6]. Before studying the limiting behaviour of the system as $\lambda\to 0$ we must remove the free part of the evolution.

The condition of the following lemma gives information about the asymptotic form of the interaction as $\lambda\to 0$. The function F need not be bounded since only bounded functions of it appear.

Lemma 2.3. *Suppose* $\lim_{\lambda\to 0} \lambda^{-2} B_\lambda(\theta) = F(\theta)$ *almost everywhere. Then for all* $x, y \in L$

$$\lim_{\lambda\to 0} e^{-iH_0 t}\alpha_{\lambda,t}\{U(x,y)\}\, e^{iH_0 t} = U(x^{(\tau)}, y^{(\tau)}) \exp[-\tfrac{1}{4} r^{(\tau)}] \tag{2.19}$$

the limit being taken in the strong operator topology, where

$$x^{(\tau)} = P\cos\left(\frac{\tau}{\omega}F\right)x - P\omega\sin\left(\frac{\tau}{\omega}F\right)y\,, \tag{2.20}$$

$$y^{(\tau)} = P\omega^{-1}\sin\left(\frac{\tau}{\omega}F\right)x + P\cos\left(\frac{\tau}{\omega}F\right)y\,, \tag{2.21}$$

$$r^{(\tau)} = \coth\left(\frac{\beta\omega}{2}\right)\{\omega^{-1}(\|x\|^2 - \|x^{(\tau)}\|^2) + \omega(\|y\|^2 - \|y^{(\tau)}\|^2)\}\,. \tag{2.22}$$

Comment. The complex form of these equations is

$$z^{(\tau)} = P\exp\left[i\frac{\tau}{\omega}F\right]z\,, \tag{2.23}$$

$$r^{(\tau)} = \coth\left(\frac{\beta\omega}{2}\right)\{\|z\|^2 - \|z^{(\tau)}\|^2\}\,. \tag{2.24}$$

Proof. Direct calculations show that

$$e^{-iH_0 t}\alpha_{\lambda,t}\{U(x,y)\}\, e^{iH_0 t} = U(u_{\lambda,t}, v_{\lambda,t}) \exp[-\tfrac{1}{4} r_{\lambda,t}] \tag{2.25}$$

where

$$u_{\lambda,t} = x_{\lambda,t}\cos(\omega t) + y_{\lambda,t}\,\omega\sin(\omega t)\,, \tag{2.26}$$

$$v_{\lambda,t} = -x_{\lambda,t}\,\omega^{-1}\sin(\omega t) + y_{\lambda,t}\cos(\omega t)\,. \tag{2.27}$$

We have to show that

$$\lim_{\lambda\to 0} u_{\lambda,t} = x^{(\tau)}; \qquad \lim_{\lambda\to 0} v_{\lambda,t} = y^{(\tau)}\,, \tag{2.28}$$

$$\lim_{\lambda\to 0} r_{\lambda,t} = r^{(\tau)}\,. \tag{2.29}$$

Substituting from Eqs. (2.5) and (2.6), with the parameter λ re-introduced, into Eq. (2.26) yields

$$\begin{aligned} u_{\lambda,t} &= \{P\cos(C_\lambda t)\,x - PC_\lambda\sin(C_\lambda t)\,y\}\cos(\omega t) \\ &\quad + \{PC_\lambda^{-1}\sin(C_\lambda t)\,x + \cos(C_\lambda t)\,y\}\,\omega\sin(\omega t) \\ &= P\cos(C_\lambda t - \omega t)\,x - P\omega\sin(C_\lambda t - \omega t)\,y \\ &\quad + P\sin(\omega t)\,(C_\lambda^{-1}\omega - 1)\sin(C_\lambda t)\,x \\ &\quad + P\cos(\omega t)\,(\omega - C_\lambda)\sin(C_\lambda t)\,y\,. \end{aligned}$$

The last two terms of this equation converge to zero in norm as $\lambda\to 0$ uniformly in t, the proof involving use of the Lebesgue dominated convergence theorem. Also

$$\lim_{\lambda\to 0} P\cos(C_\lambda t-\omega t)\,x$$
$$=\lim_{\lambda\to 0}\sum_{r=1}^{n}\sum_{s=1}^{n} e_r\langle x,e_s\rangle\,\langle\cos(C_\lambda t-\omega t)\,e_s,e_r\rangle$$
$$=\sum_{r=1}^{n}\sum_{s=1}^{n} e_r\langle x,e_s\rangle\lim_{\lambda\to 0}\frac{1}{2\pi}\int_{-\pi}^{\pi}\cos(C_\lambda(\theta)\,t-\omega t)\,e^{iN(s)\theta-iN(r)\theta}\,d\theta$$
$$=\sum_{r=1}^{n}\sum_{s=1}^{n} e_r\langle x,e_s\rangle\frac{1}{2\pi}\int_{-\pi}^{\pi}\cos\left(\frac{\tau}{\omega}F(\theta)\right)e^{iN(s)\theta-iN(r)\theta}\,d\theta$$
$$=\sum_{r=1}^{n}\sum_{s=1}^{n} e_r\langle x,e_s\rangle\left\langle\cos\left(\frac{\tau}{\omega}F\right)e_s,e_r\right\rangle$$
$$=P\cos\left(\frac{\tau}{\omega}F\right)x\,.$$

This and similar calculations yield Eq. (2.28). Now

$$r_{\lambda,t}=\left\langle C_\lambda^{-1}\coth\left(\frac{\beta C_\lambda}{2}\right)\xi_{\lambda,t},\xi_{\lambda,t}\right\rangle+\left\langle C_\lambda\coth\left(\frac{\beta C_\lambda}{2}\right)\eta_{\lambda,t},\eta_{\lambda,t}\right\rangle$$
$$=\omega^{-1}\coth\left(\frac{\beta\omega}{2}\right)\|\xi_{\lambda,t}\|^2+\omega\coth\left(\frac{\beta\omega}{2}\right)\|\eta_{\lambda,t}\|^2$$
$$+\int_{-\pi}^{\pi}\left[C_\lambda^{-1}(\theta)\coth\frac{\beta C_\lambda(\theta)}{2}-\omega^{-1}\coth\frac{\beta\omega}{2}\right]|\xi_{\lambda,t}(\theta)|^2\,d\theta$$
$$+\int_{-\pi}^{\pi}\left[C_\lambda(\theta)\coth\frac{\beta C_\lambda(\theta)}{2}-\omega\coth\frac{\beta\omega}{2}\right]|\eta_{\lambda,t}(\theta)|^2\,d\theta\,.$$

Since $\xi_{\lambda,t}(\theta)$ and $\eta_{\lambda,t}(\theta)$ are bounded uniformly in λ, t, θ and since $C_\lambda^{\pm 1}(\theta)$ are bounded uniformly in λ, θ and converge almost everywhere to $\omega^{\pm 1}$, the third and fourth terms of the above equation converge to zero uniformly in t as $\lambda\to 0$. Also

$$\omega^{-1}\|\xi_{\lambda,t}\|^2+\omega\|\eta_{\lambda,t}\|^2$$
$$=\omega^{-1}\|\cos(C_\lambda t)\,x-C_\lambda\sin(C_\lambda t)\,y-x_{\lambda,t}\|^2$$
$$+\omega\|C_\lambda^{-1}\sin(C_\lambda t)\,x+\cos(C_\lambda t)\,y-y_{\lambda,t}\|^2$$
$$=\omega^{-1}\{\|\cos(C_\lambda t)\,x-C_\lambda\sin(C_\lambda t)\,y\|^2-\|x_{\lambda,t}\|^2\}$$
$$+\omega\{\|C_\lambda^{-1}\sin(C_\lambda t)\,x+\cos(C_\lambda t)\,y\|^2-\|y_{\lambda,t}\|^2\}$$
$$=\omega^{-1}\|x\|^2+\omega\|y\|^2-\omega^{-1}\|x_{\lambda,t}\|^2-\omega\|y_{\lambda,t}\|^2$$
$$+\langle(\omega C_\lambda^{-2}-\omega^{-1})\sin^2(C_\lambda t)\,x,x\rangle$$
$$+2\langle(\omega C_\lambda^{-1}-\omega^{-1}C_\lambda)\sin(C_\lambda t)\cos(C_\lambda t)\,x,y\rangle$$
$$+\langle(\omega^{-1}C_\lambda^2-\omega)\sin^2(C_\lambda t)\,y,y\rangle\,.$$

The last three terms converge to zero uniformly in t as $\lambda \to 0$. Finally

$$\begin{aligned}&\omega^{-1}\|x_{\lambda,t}\|^2+\omega\|y_{\lambda,t}\|^2\\&=\omega^{-1}\|u_{\lambda,t}\|^2+\omega\|v_{\lambda,t}\|^2\end{aligned}$$

so substituting $t=\lambda^{-2}\tau$

$$\begin{aligned}\lim_{\lambda\to 0} r_{\lambda,t}&=\lim_{\lambda\to 0}\coth\left(\frac{\beta\omega}{2}\right)[\omega^{-1}\|x\|^2+\omega\|y\|^2-\omega^{-1}\|u_{\lambda,t}\|^2-\omega\|u_{\lambda,t}\|^2]\\&=\coth\left(\frac{\beta\omega}{2}\right)[\omega^{-1}\|x\|^2+\omega\|y\|^2-\omega^{-1}\|x^{(\tau)}\|^2-\omega\|y^{(\tau)}\|^2]\end{aligned}$$

making use of Eq. (2.28).

We now write

$$\gamma_\tau\{U(x,y)\}=U(x^{(\tau)},y^{(\tau)})\exp[-\tfrac{1}{4}r^{(\tau)}] \tag{2.30}$$

where $x, y \in L$ and $x^{(\tau)}, y^{(\tau)}, r^{(\tau)}$ are defined as in Lemma (2.3). The quantum system is said to exhibit Markov behaviour if

$$\gamma_{\sigma+\tau}=\gamma_\sigma\gamma_\tau \tag{2.31}$$

for all $\sigma, \tau \geqq 0$. This will not generally be true, but there exist a variety of interactions for which it does hold, one being provided by the following theorem.

Theorem 2.4. *There exists an interaction $a_n^{(\lambda)}$ depending on λ such that if*

$$B_\lambda(\theta)=\sum_{n=-\infty}^{\infty} a_n^{(\lambda)} e^{in\theta} \tag{2.32}$$

then

$$\lim_{\lambda\to 0}\lambda^{-2}B_\lambda(\theta)=k\cot|\theta|+h \tag{2.33}$$

for all $\theta \in (-\pi, \pi)$ except $\theta=0$. The quantum system consisting of any single oscillator exhibits Markov behaviour for this interaction in the limit $\lambda \to 0$. The quantum system consisting of any pair of oscillators does not generally exhibit Markov behaviour.

Proof. We define

$$B_\lambda(\theta)=\lambda^2 k\cos\theta\{1+\lambda^2-\cos^2\theta\}^{-\frac{1}{2}}+\lambda^2 h \tag{2.34}$$

where k and h are arbitrary real numbers. Since $B_\lambda(\theta)$ is continuously differentiable and periodic its Fourier coefficients satisfy Eq. (1.4) for all $\lambda>0$. Since

$$|B_\lambda(\theta)| \leqq \lambda|k|+\lambda^2|h|\,.$$

Eq. (1.10) is satisfied at least for λ sufficiently small. Eq. (2.33) may be easily verified.

We first treat the case of a single oscillator. We take $e(\theta)=(2\pi)^{-\frac{1}{2}}$ and let L be the one-dimensional subspace of M generated by e. Eq. (2.23) becomes

$$z^{(\tau)}=f(\tau)\,z \tag{2.35}$$

where

$$\begin{aligned} f(\tau)&=\left\langle \exp\left[i\frac{\tau}{\omega}F\right]e,e\right\rangle \\ &=\frac{1}{2\pi}\int_{-\pi}^{\pi}\exp\left[i\frac{\tau}{\omega}k\cot|\theta|+i\frac{\tau}{\omega}h\right]d\theta \\ &=\exp\left[i\frac{\tau}{\omega}h-|k|\frac{\tau}{\omega}\right] \end{aligned} \tag{2.36}$$

by elementary calculations. It follows that

$$r^{(\tau)}=\coth\left(\frac{\beta\omega}{2}\right)|z|^2\left\{1-\exp\left[-2|k|\frac{\tau}{\omega}\right]\right\} \tag{2.37}$$

Eq. (2.30) may now be verified by direct calculation.

We now consider the system consisting of a pair of oscillators. We let

$$e_1(\theta)=\frac{1}{\sqrt{2\pi}};\qquad e_2(\theta)=\frac{e^{in\theta}}{\sqrt{2\pi}}$$

and let L be the subspace of M generated by e_1 and e_2. If an arbitrary vector $z\in L$ is written in the form $z=z_1e_1+z_2e_2$ where $z_i\in\mathbb{C}$ then

$$z_i^{(\tau)}=f_{i1}(\tau)\,z_1+f_{i2}(\tau)\,z_2$$

where

$$\begin{aligned} f_{ij}(\tau)&=\left\langle \exp\left[i\frac{\tau}{\omega}F\right]e_j,e_i\right\rangle \\ &=\int_{-\pi}^{\pi}\exp\left[i\frac{\tau}{\omega}k\cot|\theta|+i\frac{\tau}{\omega}h\right]e_j(\theta)\,\overline{e_i(\theta)}\,d\theta\,. \end{aligned}$$

In case $i=j$ this has already been calculated. Also

$$f_{12}(\tau)=f_{21}(\tau)=\frac{1}{2\pi}\exp\left[\frac{i\tau h}{\omega}\right]\int_{-\pi}^{\pi}\exp\left[i\frac{\tau}{\omega}\mathrm{k}\cot|\theta|+in\theta\right]d\theta\,.$$

This can be calculated in terms of elementary functions if the oscillators have an even separation. If $n=2m$ one obtains

$$f_{12}(\tau)=-\frac{\tau|k|}{m\omega}L^1_{m-1}\left(\frac{2\tau|k|}{\omega}\right)\exp\left[\frac{i\tau h}{\omega}-\frac{\tau|k|}{\omega}\right]$$

where L^1_{m-1} is the symbol for a Laguerre polynomial. It is clear that the system does not then have Markov behaviour.

§ 3. The Pauli Master Equation

Throughout this section we consider exclusively the particular interaction defined in Theorem 4.2. Moreover we take the system to consist of the single oscillator chosen in the proof. In order to proceed to a derivation of the Pauli master equation we fix the Hilbert space on which the Weyl operators corresponding to the chosen oscillator act. Let $\mathscr{H} = L^2(\mathbb{R})$ and let

$$\{\phi_0(e)\, f\}\,(x) = \omega^{-\frac{1}{2}} x f(x)\,, \tag{3.1}$$

$$\{\pi_0(e)\, f\}\,(x) = -i\omega^{\frac{1}{2}} f'(x)\,. \tag{3.2}$$

Then define

$$U(x, y) = \exp\{ix\phi_0(e) + iy\pi_0(e)\} \tag{3.3}$$

for arbitrary real number x and y. Let V denote the space of all self-adjoint trace class operators on $\mathscr{H}$. If an operator $\varrho \in V$ has spectral decomposition

$$\varrho = \sum_{n=1}^{\infty} \lambda_n \xi_n \otimes \bar{\xi}_n \tag{3.4}$$

where $\{\xi_n\}_{n=1}^{\infty}$ is an orthonormal basis of $\mathscr{H}$ and if we define the trace norm by

$$\|\varrho\| = \sum_{n=1}^{\infty} |\lambda_n| \tag{3.5}$$

then V becomes a Banach space under the trace norm [7].

The following proposition transforms the results of the last section into the Schrodinger representation. Its proof involves some general abstract arguments which we postpone to the next section, but the crucial semigroup property is a consequence of the calculations already performed.

Proposition 3.1. *There exists a strongly continuous one-parameter semigroup of linear maps $T_\tau : V \to V$ defined for all $\tau \geqq 0$, such that*

(i) *if* $\varrho \geqq 0$ *then* $T_\tau(\varrho) \geqq 0$; (3.6)

(ii) $\mathrm{tr}[T_\tau(\varrho)] = \mathrm{tr}[\varrho]$ *for all* $\varrho \in V$; (3.7)

(iii) $\mathrm{tr}[T_\tau(\varrho)\, U(x, y)] = \mathrm{tr}[\varrho \gamma_\tau\{U(x, y)\}]$ (3.8)

for all $x, y \in \mathbb{R}$, $\tau \geqq 0$ and $\varrho \in V$.

We comment that such semigroups have been extensively studied in the context of quantum stochastic processes [8–10] and that the zero temperature case of this semigroup occurred in [11].

This proposition is a lot stronger than the Pauli master equation as described by van Hove [6]. In this context the Pauli master equation only describes the energy density evolution while this proposition allows calculations concerning the time evolution of the distribution of any state with respect to any observable.

To derive the Pauli master equation we take the usual harmonic oscillator Hamiltonian, namely

$$H_0 = \tfrac{1}{2}\{\pi(e)^2 + \omega^2 \phi(e)^2 - \omega\} \tag{3.9}$$

and let $\{e_n\}_{n=0}^{\infty}$ be its normalised eigenvectors, so that

$$H_0 e_n = n\omega e_n , \tag{3.10}$$

for $n = 0, 1, 2, \ldots$ We start by describing the evolution under T_τ of states ϱ of a particular form.

Proposition 3.2. *Let $\varrho_s \in V$ be defined for all $s > 0$ by*

$$\varrho_s = (1 - e^{-s\omega})\, e^{-sH_0} . \tag{3.11}$$

Then for all $s > 0$ and $\tau \geqq 0$

$$T_\tau(\varrho_s) = \varrho_{s(\tau)} \tag{3.12}$$

where

$$\coth\left(\frac{\omega s(\tau)}{2}\right) = e^{-2|k|\tau/\omega} \coth\left(\frac{\omega s}{2}\right) + (1 - e^{-2|k|\tau/\omega}) \coth\left(\frac{\omega\beta}{2}\right). \tag{3.13}$$

For all $s > 0$

$$\lim_{\tau \to \infty} T_\tau(\varrho_s) = \varrho_\beta \tag{3.14}$$

the limit being taken in the trace norm.

Proof. We quote a formula proved in the appendix to [2], namely

$$\operatorname{tr}[\varrho_s U(x, y)] = \exp\left[-\frac{1}{4} \coth\left(\frac{\omega s}{2}\right) \{\omega^{-1} x^2 + \omega y^2\}\right] \tag{3.15}$$

and use it to make the following calculations.

$$\begin{aligned}
\operatorname{tr}[T_\tau(\varrho_s)\, U(x, y)] &= \operatorname{tr}[\varrho_s \gamma_\tau\{U(x, y)\}] \\
&= \operatorname{tr}[\varrho_s U(x^{(\tau)}, y^{(\tau)})] \exp\left[-\frac{1}{4} r^{(\tau)}\right] \\
&= \exp\left[-\frac{1}{4} \coth\left(\frac{\omega s}{2}\right) \{\omega^{-1} x^{(\tau)2} + \omega y^{(\tau)2}\} - \frac{1}{4} r^{(\tau)}\right] \\
&= \exp\left[-\frac{1}{4} \coth\left(\frac{\omega s}{2}\right) \{\omega^{-1} x^2 + \omega y^2\}\, e^{-2|k|\tau/\omega} - \frac{1}{4} r^{(\tau)}\right] \\
&= \exp\left[-\frac{1}{4} \coth\left(\frac{\omega s(\tau)}{2}\right) \{\omega^{-1} x^2 + \omega y^2\}\right] \\
&= \operatorname{tr}[\varrho_{s(\tau)} U(x, y)] .
\end{aligned}$$

Since linear combinations of the operators $U(x, y)$ are strongly dense in $\mathscr{L}(\mathscr{H})$, Eq. (3.12) follows. Eq. (3.14) is a consequence of the result

$$\lim_{\tau\to\infty} s(\tau) = \beta\,. \tag{3.16}$$

In order to state the Pauli master equation we note that the positive normalised states which commute with H_0 are precisely those which can be written in the form

$$\varrho = \sum_{n=0}^{\infty} \varrho_n e_n \otimes \bar{e}_n \tag{3.17}$$

where $\varrho_n \geqq 0$ for all n and $\sum_{n=0}^{\infty} \varrho_n = 1$.

Theorem 3.3. *If ϱ is a positive normalised state which commutes with with H_0 then $T_\tau(\varrho)$ commutes H_0 for all $\tau \geqq 0$, so that*

$$T_\tau(\varrho) = \sum_{n=0}^{\infty} \varrho_n^{(\tau)} e_n \otimes \bar{e}_n \tag{3.18}$$

where $\varrho_n^{(\tau)} \geqq 0$ and $\sum_{n=0}^{\infty} \varrho_n^{(\tau)} = 1$. The coefficients $\varrho_n^{(\tau)}$ can be calculated from the equation

$$\varrho_m^{(\tau)} = \sum_{n=0}^{\infty} P_{mn}^{(\tau)} \varrho_n \tag{3.19}$$

where $P_{mn}^{(\tau)}$ are the coefficients of a continuous time classical Markov process. This process is ergodic and for all integers m, n we have

$$\lim_{\tau\to\infty} P_{mn}^{(\tau)} = (1 - e^{-\beta\omega})\, e^{-m\beta\omega}\,. \tag{3.20}$$

Proof. The first statement of the theorem is a consequence of the fact that linear combinations of states of the form ϱ_s given in Proposition (3.2) are dense in the space of all states which commute with H_0. The remainder of the theorem is then no more than a translation of the results we have obtained into the language of classical probability theory.

We commented earlier that before going to the limit $\lambda \to 0$ we had to remove the free part of the evolution, and this was done in Eq. (2.19). If one is only interested in the evolution of the energy density then this is not necessary because the free evolution does not affect the energy density. This modification makes our result more obviously similar to that obtained by van Hove [6].

The equations we have obtained for a quantum oscillator have already been studied by Schwinger [12], but he did not justify them by reference to the dynamics of an infinite system.

§ 4. The General Framework

We discuss finally the calculations of the earlier sections from a more general point of view. The purpose of this is to clarify the nature of the operation M introduced in Section 2, and to prove Proposition (3.1). The abstract setting consists of an adaptation of a part of the theory of quantum stochastic processes to a C^*-algebra context.

We let $\mathscr{B}$ be the C^*-algebra of the canonical commutation relations over the real Hilbert space M, so that $U: M \times M \to \mathscr{B}$ is a map such that $U(f_1, f_2)$ is unitary for all $f_1, f_2 \in M$ and

$$U(f_1,f_2)U(g_1,g_2) = U(f_1+g_1,f_2+g_2)\exp\left[\frac{i}{2}(\langle f_2,g_1\rangle - \langle f_1,g_2\rangle)\right] \quad (4.1)$$

and $\mathscr{B}$ is the norm closure of the linear space generated by all $U(f, g)$ where $f, g \in M$. It has been shown by Slawny [13] that this algebra is independent of the representation of the canonical commutation relations chosen. If ϕ is a state of $\mathscr{B}$, then ϕ defines a map

$$E_\phi : M \times M \to \mathbb{C} \quad (4.2)$$

by

$$E_\phi(f, g) = \langle \phi, U(f, g)\rangle . \quad (4.3)$$

This map is called the *expectation function* of the state ϕ and completely determines ϕ. It was shown by Araki and Segal [14, 15] that these expectation functions can be characterised by simple algebraic properties which we do not write down here.

Now let L be an n-dimensional subspace of M and let $\mathscr{A}$ be the associated C^*-subalgebra of $\mathscr{B}$, so that $\mathscr{A}$ is generated by

$$\{U(x, y) : x, y \in L\} . \quad (4.4)$$

Slawny's results allow us to realise $\mathscr{A}$ concretely on $\mathscr{H} = L^2(\mathbb{R}^n)$. If V is the Banach space of self-adjoint trace class operators on $\mathscr{H}$ and $\varrho \in V^+$ has trace one then

$$E_\varrho(x, y) = \mathrm{tr}[\varrho U(x, y)] \quad (4.5)$$

is an expectation function on $L \times L$.

We include the following well-known result for the sake of completeness.

Proposition 4.1. *Let ϕ be a state on $\mathscr{A}$. Then there exists a trace class operator $\varrho \in V^+$ such that*

$$\langle \phi, A\rangle = \mathrm{tr}[\varrho A] \quad (4.6)$$

for all $A \in \mathscr{A}$ if and only if the expectation function $E_\phi : L \times L \to \mathbb{C}$ is continuous.

Proof. The state ϕ gives rise to a cyclic representation of the Weyl group by means of the Gelfand-Segal construction. This representation is strongly continuous if and only if the function E_ϕ is continuous. The proposition is now merely a reformulation of von Neumann's uniqueness theorem [15, 16] for strongly continuous representations of the Weyl group.

The proposition allows us to regard the space V of trace class operators as a subspace of $\mathscr{A}^*$ and we shall make this identification from now on.

Proposition 4.2. *Let $K:\mathscr{A}\to\mathscr{A}$ be a positive linear map such that $K(1)=1$ and such that for all $\psi\in\mathscr{H}$ the function*

$$x, y \to \langle K\{U(x,y)\}\psi, \psi\rangle \tag{4.7}$$

is continuous on $L\times L$. Then the adjoint map $K^*:\mathscr{A}^*\to\mathscr{A}^*$ maps V into V and K can be extended to an ultraweakly continuous positive linear map $\bar{K}:\mathscr{L}(\mathscr{H})\to\mathscr{L}(\mathscr{H})$.

Proof. If $\varrho\in V$ is given by Eq. (3.4) then

$$\begin{aligned}\langle K^*(\varrho), U(x,y)\rangle &= \langle \varrho, K\{U(x,y)\}\rangle \\ &= \sum_{n=1}^{\infty} \lambda_n \langle K\{U(x,y)\}\xi_n, \xi_n\rangle\end{aligned}$$

which is easily seen to be a continuous function of x and y. Proposition (4.1) now implies that $K^*(\varrho)\in V$. We now let $H: V\to V$ be the restriction of K^* to V and recall, [7], that V^* can be identified with $\mathscr{L}_s(\mathscr{H})$, the space of self-adjoint bounded operators on $\mathscr{H}$. If we define $\bar{K}=H^*$, the remaining statements of the proposition follow.

Proposition 4.3. *Suppose that $\varrho\in V^+$ and $\varrho_n\in V^+$ for $n=1,2,3,\ldots$ Then*

$$\lim_{n\to\infty} \operatorname{tr}[\varrho_n A] = \operatorname{tr}[\varrho A] \tag{4.8}$$

for all $A\in\mathscr{A}$ if and only if

$$\lim_{n\to\infty} \|\varrho-\varrho_n\| = 0, \tag{4.9}$$

the norm being the trace norm.

Proof. That the second condition implies the first is a simple consequence of the inequality

$$|\operatorname{tr}[\varrho_n A] - \operatorname{tr}[\varrho A]| \leqq \|\varrho-\varrho_n\|\,\|A\|\,.$$

Conversely let A be any bounded operator of the form

$$A = \int_L \int_L f(x,y)\, U(x,y)\, d^n x\, d^n y \tag{4.10}$$

where f is any continuous function of compact support. We comment that $A \notin \mathscr{A}$ because $x, y \to U(x, y)$ is not norm continuous, but the integral can be defined in the ultraweak sense. Then

$$\begin{aligned}\lim_{n\to\infty} \operatorname{tr}[\varrho_n A] &= \lim_{n\to\infty} \iint f(x, y) \operatorname{tr}[\varrho_n U(x, y)]\, dx\, dy \\ &= \iint f(x, y) \operatorname{tr}[\varrho U(x, y)]\, dx\, dy \\ &= \operatorname{tr}[\varrho A],\end{aligned}$$

these calculations being justified by Lebesgue's dominated convergence theorem.

Writing A as an integral operator we see that it is compact and that operators of the form of Eq. (4.10) are norm dense in the set of all compact operators. Therefore

$$\lim_{n\to\infty} \operatorname{tr}[\varrho_n A] = \operatorname{tr}[\varrho A] \tag{4.11}$$

for all compact operators A on $\mathscr{H}$, and ϱ_n converges to ϱ in the weak operator topology. The result now follows by [8] upon the observation that since $t \in \mathscr{A}$

$$\lim_{n\to\infty} \operatorname{tr}[\varrho_n] = \operatorname{tr}[\varrho]\,. \tag{4.12}$$

The following proposition provides a clarification at the C^*-algebra level of the nature of the operation M introduced in Section 2 and of the maps α_t defined on the Weyl operators of a finite number of degrees of freedom.

Proposition 4.4. *There exists a unique positive linear map* $\alpha_t : \mathscr{A} \to \mathscr{A}$ *such that* $\alpha_t(1) = 1$ *and*

$$\alpha_t\{U(x, y)\} = U(x_t, y_t) \exp[-\tfrac{1}{4} r_t] \tag{4.13}$$

for all $x, y \in L$ *and all* $t \geqq 0$, *where* x_t, y_t, r_t *are defined as in Lemma* (2.1).

Proof. We define a positive linear map $N : \mathscr{A}^* \to \mathscr{B}^*$ by making use of the expectation function of the thermal equilibrium state E_β. If $\phi \in \mathscr{A}^{*+}$ and P is the projection of M onto L then we define

$$E_{N\phi}(f, g) = E_\phi(Pf, Pg)\, E_\beta((1-P) f, (1-P) g) \tag{4.14}$$

for all $f, g \in M$. $E_{N\phi}$ satisfies the condition of Araki and Segal, [14, 15], and so is the expectation function of a state $N\phi \in \mathscr{B}^{*+}$. The linearity of the map $N : \mathscr{A}^* \to \mathscr{B}^*$ is easily proved. The adjoint map $N^* \mathscr{B}^{**} \to \mathscr{A}^{**}$ is positive, linear and

$$N^*\{U(f, g)\} = U(Pf, Pg)\, E_\beta((1-P) f, (1-P) g) \tag{4.15}$$

by direct calculation. Since operators of the form $U(f, g)$ generate $\mathscr{B}$ in the norm topology, and since N^* is norm continuous we can conclude that $N^*(\mathscr{B}) \subseteq \mathscr{A}$. We comment in passing that the restriction M of N^* to $\mathscr{B}$ is a conditional expectation of $\mathscr{B}$ onto $\mathscr{A}$, [17].

There exists an automorphism group θ_t of $\mathscr{B}$ such that in the Fock representation

$$\theta_t(B) = e^{iHt} B e^{-iHt} \tag{4.16}$$

for all $B \in \mathscr{B}$, and for Weyl operators one has

$$\theta_t\{U(f, g)\} = U(f_t, g_t) \tag{4.17}$$

where

$$f_t = \cos(Ct)\, f - C \sin(Ct)\, g \tag{4.18}$$

and

$$g_t = C^{-1} \sin(Ct)\, f + \cos(Ct)\, g\,. \tag{4.19}$$

If now we define $\alpha_t : \mathscr{A} \to \mathscr{A}$ by

$$\alpha_t(A) = M\{\theta_t(A)\}$$

then it is immediate that α_t is a positive linear map and satisfies Eq. (4.13).

We are now in a position to give *Proof of Proposition* (3.1).

We have shown in Lemma (2.3) that

$$\lim_{\lambda \to 0} e^{-iH_0 t} \alpha_{\lambda, t}(A)\, e^{iH_0 t} = \gamma_\tau(A)$$

for all Weyl operators $A = U(x, y)$ where $x, y \in L$, the limit being taken in the strong operator topology and lying in $\mathscr{A}$. General linearity and density arguments now imply that the limit exists in the strong operator topology, and lies in $\mathscr{A}$, for all $A \in \mathscr{A}$. Since a strong limit of positive maps is positive it follows that $\gamma_\tau : \mathscr{A} \to \mathscr{A}$ is a positive linear mapping. We now define $T_\tau : \mathscr{A}^* \to \mathscr{A}^*$ by $T_\tau = \gamma_\tau^*$ so that T_τ is positive and linear. That T_τ taken V into V is a consequence of Proposition (4.2) together with the explicit formulae of Lemma (2.3). The strong continuity of the map $\tau \to T_\tau$ follows by Proposition (4.3) while all the other statements are easy consequences of the duality formula $T_\tau = \gamma_\tau^*$.

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